

Ethyl ethylcarbamate
623-78-9 | DTXSID0060775

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 2.65e-01 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.78e-01

Confidence level: 8.01e-01

Nearest Neighbors from the Training Set

Image not found

Methyl nicotinate

Measured: 3.47e-01

Predicted: 4.31e-01

Image not found

Carbamic acid, diethyl-, methyl ester

Measured: 5.11e-01

Predicted: 3.83e-01

Image not found

Ethyl nicotinate

Measured: 3.70e-01

Predicted: 2.90e-01

Image not found

2-Chloro-1-(chloromethyl)ethyl carbamate

Measured: 4.36e-02

Predicted: 3.91e-02